COMPONENTS:	EVALUATOR:
<pre>(1) o-Xylene; C₈H₁₀; [95-47-6] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

CRITICAL EVALUATION:

Quantitative solubility data for the o-xylene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies ofthe o-Xylene (1) - Water (2) System

Reference	Т/К	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Guseva and Parnov (ref 2)	385-524	(1) in (2)	unspecified
McAuliffe (ref 3)	298	(l) in (2)	GLC
Hoegfeldt and Bolander (ref 4)	298	(2) in (1)	Karl Fischer
Polak and Lu (ref 6)	273,298	mutual	GLC, Karl Fischer
Sutton and Calder (ref 7)	298	(1) in (2)	GLC
Price (ref 8)	298	(l) in (2)	GLC
Krzyzanowska and Szeliga (ref 9)	298	(1) in (2)	GLC
Sanemasa $et \ al.$ (ref 10)	299-318	(1) in (2)	spectrophotometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Alwani and Schneider (ref 5) have also reported data on a critical locus at high temperatures and pressures. For convenience further discussion of this system will be given in two parts.

1. SOLUBILITY OF O-XYLENE (1) IN WATER (2)

The high temperature, high pressure data of Guseva and Parnov (ref 2) and Alwani and Schneider (ref 5) have been obtained under quite different conditions and thus no Critical Evaluation of their data is possible. However, it may be noted that the data of Guseva and Parnov are frequently unreliable. The interested user is referred to the relevant Data Sheets for experimental values.

At atmospheric pressure all the available data are listed in Table 2 except for the value of Krzyzanowska and Szeliga (ref 9) which does not appear to be independent of that of Price (ref 8) and has therefore been excluded from consideration.



(continued next page)

COMPONENTS:	EVALUATOR:	
<pre>(1) o-Xylene; C₈H₁₀; [95-47-6] (2) Water; H₂O; [7732-18-5]</pre>	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.	
	July 1985	

CRITICAL EVALUATION: (continued)

At 298K, the data of McAuliffe (ref 3), Sutton and Calder (ref 7), Price (ref 8) and Sanemasa *et al.* (ref 10) are in excellent agreement and their average is Recommended. The values of Andrews and Keefer (ref 1) and Polak and Lu (ref 6) are markedly higher ($>3\sigma_n$) and are rejected.

At other temperatures only the data of Sanemasa $et \ all$. (ref 10) are available except for the 273K datum of Polak and Ly (ref 6). These data are therefore regarded as Tentative.

Selected data are plotted in Figure 1.

TABLE 2: Recommended (R) and Tentative Solubility Values ofo-Xylene (1) in Water (2)

<i>Т/</i> К	Solubility Reported values 10 ² g(1)/100g sln	values "Best" values (10 ² g(l)/100g sln	± σ _n) ^α 10 ⁵ ∞ ₁
273 1.42	2 (ref 5)	1.4	2.4
288 1.6	8 (ref 10)	1.7	2.9
298 1.7 1.6	5 (ref 3), 1.705 (ref 7), 7 (ref 8), 1.79 (ref 10)	1.73 ± 0.05 (R)	2.93 (R)
308 1.98	8 (ref 10)	2.0	3.4
318 2.14	4 (ref 10)	2.1	3.6

a Obtained by averaging where appropriate; $\sigma_{\rm n}$ has no statistical significance.

(continued next page)

COMPONENTS: EVALUATOR: (1) o-Xylene; C₈H₁₀; [95-47-6] G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch (2) Water; H₂O; [7732-18-5] University, Perth, W.A., Australia. July 1985 (continued) CRITICAL EVALUATION: REFERENCES 1. Andrews, L.J.; Keefer, R.M. J. Am. Chem. Soc. 1949, 71, 3644-7. Guseva, A.N.; Parnov, E.I. Vestn. Mosk. Univ. Khim. 1963, 18, 76-9. 2. 3. McAuliffe, C. Nature 1963, 200, 1092-3; J. Phys. Chem. 1966, 70, 1267-72. 4. Hoegfeldt, E.; Bolander, B. Ark. Kemi 1964, 21, 161-86. Alwani, Z.; Schneider, G.M. Ber. Bunsenges. 1969, 73, 294-301. 5. Polak, J.; Lu, B. C-Y. Can. J. Chem. 1973, 51, 4018-23. 6. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2. 7. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44; see also Ph.D. Dissertation, 1973, Univ. California, Riverside, CA, U.S.A., 8. quoted in ref 10. Krzyzanowska, T.; Szeliga, J. Nafta (Katowice) 1978, 34, 413-7. 9. Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. <u>1982</u>, 55, 1054-62. 10. ACKNOWLEDGEMENT The Evaluator thanks Dr Brian Clare for the graphics.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	Andrews, L.J.; Keefer, R.M.
(2) Water; H ₂ O; [7732-18-5]	J. Am. Chem. Soc. <u>1949</u> , 71, 3644-77.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of o-Xylene in water at 0.0204 g(l)/100 g sln.	t 25°C was reported to be
The corresponding mole fraction, x_1 , x_3 .46 x 10^{-5} .	calculated by the compilers is
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was rotated for twenty hours in a constant tem-	(1) Eastman Kodak Co. best grade; fractionally distilled; b.p.
(5-20 mL) of the aqueous phase was	range 144.3-144.5°C.
measured volume of hexane (10-50 mL)	(2) Not specified.
Erlenmeyer flask. Next, the absorb-	
ured against a hexane blank on the Beckman spectrophotomoter	
beckhan spectrophotometer.	POTTMATED PDDADA
	Not specified.
	REFERENCES:

COMPONENTS:			ORIGINAL MEASUREMENTS:	
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]			Guseva, A.N.; Parnov, E.I.	
(2) Water; H ₂ O; [7732-18-5]		8-5]	Vestn. Mosk. Univ. Khim. <u>1963</u> , 18, 76-9.	
VARIABLES:		<u> </u>	PREPARED BY:	
_				
Temperature:	139-251°C		A. Maczynski and Z. Maczynska	
EXPERIMENTAL VALUES	<u>. </u>			
	Sol	ubility of o-:	xylene in water	
	t/°C	g(l)/100 g :	sln 10 ⁴ x ₁ (compiler)	
	139	0.047	0.80	
	162	0.093	1.58	
	207 251	0.407	16.42	
			······	
		AUXILIARY	INFORMATION	
METHOD APPARATUS /PI	ROCEDURE :		SOURCE AND PURITY OF MATERIALS.	
		ada du		
sealed glass to	ts were ma ubes. No	ade in details	(1) source not specified;	
were reported	in the pap	per.	n _D , 1.5054.	
			(2) doubly distilled.	
			ESTIMATED ERROR:	
			not specified.	
			REFERENCES:	

COMPONENTS :	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	McAuliffe, C.
(2) Water; H ₂ O; [7732-18-5]	Nature (London) <u>1963</u> , 200, 1092-3.
-	
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of o-Xylene in water at	z 25°C was reported to be
0.0175 g(1)/100 g sln.	
The corresponding mole fraction, x_1 , c_1	calculated by the compilers is
2.97 x 10 .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solution of (1) in (2) was prepared by either shaking vigor-	(1) Phillips Petroleum Co.; 99+%; used as received.
ously on a reciprocal shaker or stir-	
stirrer. A 0.05 mL or 0.10 mL sample	(2) Distilled.
of the hydrocarbon-saturated water	
liquid chromatograph.	
	ESTIMATED ERROR:
	Temp. ±1.5°C
	Soly. 0.0008 (std. dev. of mean)
	REFERENCES :
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ORIGINAL MEASUREMENTS: COMPONENTS: o-Xylene; C₈H₁₀; [95-47-6] Hoegfeldt, E.; Bolander, B. (1) Water; H₂O; [7732-18-5] Ark. Kemi, 1964, 21, 161-86. (2) VARIABLES: PREPARED BY: One temperature: 25°C A. Maczynski and Z. Maczynska EXPERIMENTAL VALUES: The solubility of water in o-Xylene was reported to be 0.022 mol(2) L sln. The corresponding mass percent and mol fraction,  $x_2$ , calculated by the compilers are 0.045 g(2)/100 g sln and 0.0026. The assumption that 1.00 L sln = 876 g sln was used in the calculation. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The water determination was carried (1) Fluka; 0.7% of (m-p) xylene, out according to Johansson's modifi-cation of the Karl Fischer titration 0.07% of ethylbenzene; purity 99.0%; used as received. in ref 1, 2. ESTIMATED ERROR: Temp. ±0.3 C Soly. ±0,002 mol(2) L⁻¹ sln (type of error not specified) **REFERENCES:** 1. Hardy, C.J.; Greenfield, B.F.; Scargill, D. J. Chem. Soc. 1961, 90. 2. Johansson, A. Sv. Papperstidn. 1947, 11B, 124.

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COMPONENTS:		ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]		Polak, J.; Lu, B.CY.
(2) Water; H ₂ O; [7732-18-5]		Can. J. Chem. <u>1973</u> , 51, 4018-23.
	-	
VARIABLES:		PREPARED BY:
Temperature:	0-25°C	A. Maczynski and Z. Maczynska
		·
EXPERIMENTAL VAN	.UES:	
	Solubility	of o-xylene in water
t/°C	mg(l)/kg(2)	$g(1)/100 g sln 10^{5}x_{1}$
0(a)	142(c)	0.0142 2.41 0.0232 3.61
25 (D)	213(C)	0.0215 5.01
	Solubility	of water in o-xylene
t/°C	mg(2)/kg(1)	$g(2)/100 g sln = 10^{3}x_{2}$
0(a) 25(b)	185(a)	0.0185 1.09
25(0)	450(e)	0.0450 2.00
a∼e See "Est:	imated Error"	
	AUX	XILIARY INFORMATION
METHOD /APPARATUS	S/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis. The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas		ether (1) Eastman Organics, pure grade iL reagent; shaken three times with distilled water. (2) distilled. irred t in 7 n ESTIMATED ERROR: (2) distilled.
		$\begin{array}{c ccccccccccccccccccccccccccccccccccc$
chromatograp	hy.	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	Sutton, C.; Calder, J.A.
(2) Water; H ₂ O; [7732-18-5]	J. Chem. Eng. Data 1975, 20, 320-2.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska
EXPERIMENTAL VALUES:	
The solubility of o-xylene in water a	at 25°C was reported to be
170.5 mg(l)/kg(2). The corresponding	g mass percent and mole fraction,
$x_1$ , calculated by the compilers are (	).01705 g(1)/100 g sln and
$2.892 \times 10^{-5}$ .	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The concentration of (1) in (2) was determined by gas chroma-	SOURCE AND PURITY OF MATERIALS: (1) Aldrich Chemical Co. or Matheson Coleman and Bell
tography.	99+%.
	(2) distilled.
	ESTIMATED ERRORA
	temp. $\pm$ 0.1°C solv. 2.5 mg(1)/kg(2)
	(the standard deviation of the mean for six replicates)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [97-47-6]	Krzyzanowska, T.; Szeliga, J.
(2) Water; H ₂ O; [7732-18-5]	Nafta (Katowice), <u>1978</u> , 12, 413-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson
EVERDIVENTAL VALUES.	I
EATENINE VALUES.	
The solubility of o-xylene in water	at 25°C was reported
to be 167.0 mg(1)/kg(2).	
The corresponding mass percent and m	ole fraction, $x_1$ , calculated
by compiler are 0.0167 g(l)/100 g sl	n and 2.83 x $10^{-5}$ .
	a star at the budrogerbon water
Editor's Note: Based on the results	for this and other hydrocarbon-water bether the datum compiled here is
independent of that of Price for the	same system (see previous page).
Independent of end of a	-
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AUXILIARY	INFORMATION
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways.	(1) not specified.
First, 200 µL of (1) was injected	(2) not specified.
at 25°C. Second, the mixture of (1)	
at 70°C and then cooled to 25°C. The	e
time required to obtain equilibrium was three weeks. The solubility of	
(1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromat-	
ograph equipped with a 100-150 mesh Porasil column (70°C) and a flame	ESTIMATED ERROR:
ionization detector was used. Sat-	
were used as standard solutions.	deviation from 7-9 determinations).
	REFERENCES :
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COMPONENTS:		ORIGINAL MEASUREMENTS:	
(1) <i>o</i> -Xylene; C ₈ H ₁₀ ; [97-47-6] (2) Water; H ₂ O; [7732-18-5]		Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. <i>Bull. Chem. Soc. Jpn.</i> <u>1982</u> , 55, 1054-62.	
VARIABLES:		PREPARED BY:	
Temperature:	15-45°C	G.T. Hefter	
EXPERIMENTAL VAL	UES:	L	
	The solubility of a	o-xylene in water	
t /°C	10 ³ mol(1)/dm ³ sln	g(1)/100 g sln (compiler) ^a	$10^5 x_1$ (compiler) ^a
15	1 58 + 0 11	0 0168	2.85
25	$1.68 \pm 0.06$	0.0179	3.04
35	$1.85 \pm 0.02$	0.0198	3.35
45	$2.00 \pm 0.02$	0.0214	3.64
	AUXILIARY	INFORMATION	
METHOD/APPARATUS	/PROCEDURE:	SOURCE AND PURITY OF MAT	ERIALS:
The apparatus earlier desig described in 100-200 cm ³ o liquid (1) we but connected After thermal lished a reci was used to v to transport containing (2 were withdraw	is similar to an n (ref 2) and is detail in the paper. f (2) and 10-20 cm ³ of re placed in separate thermostatted flasks. equilibrium was estab- rculating stream of air aporize liquid (1) and the vapor to the flask ). Five 10 cm ³ aliquots n into separatory	<ul> <li>(1) Analytical reag Pure Chemical I purity 98.0%, u further purific</li> <li>(2) Redistilled; no given.</li> </ul>	ent grade (Wako ind. Ltd.), stated ised without ation. further details
funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV- spectrophotometry. Standards for the spectrophotometry were prepared by		ESTIMATED ERROR: soly. see table, typ specified. temp. ± 0.1°C.	e of error not
werdur rrow b	are IIquid Solučes.	REFERENCES: 1. Kell, G.S. J. Chem. Eng. Data 2. Sanemasa, I.; Ar	<u>1975</u> , 20, 97. Taki, M.;
]		Deguchi, Y.; Nag Chem. Lett. <u>1981</u> ,	a1, H. 225-8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C ₈ H ₁₀ ; [95-47-6]	Sutton, C.; Calder, J.A.
(2) Artificial seawater (ref 1)	J. Chem. Eng. Data <u>1975</u> , 20, 320-2.
VARIABLES:	PREPARED BY:
One salinity: 34.5 g salts/kg sln	M. Kleinschmidt
EXPERIMENTAL VALUES:	
The solubility of o-xylene in artificial seawater is reported to be	
129.6 $mg(1)/kg$ sln. The corresponding mass percent and mole fraction,	
$r_{\rm ent}$ entry based by the compiler are 0.01296 g(1)/100 g cln and 2.26 x $10^{-5}$	
$x_1$ calculated by the compiler are 0.01296 g(1)/100 g sin and 2.26 x 10	
assuming the artificial seawater composition of ref 1.	
AUXILIARY INFORMATION	
METHOD / APPARATUS / PROCEDURE :	SOURCE AND PURITY OF MATERIALS:
A test tube containing (1) was placed in a flask containing (2)	(1) from either Aldrich Chemical Co. or Matheson Coleman and
thus allowing for equilibration	Bell, 99+% pure.
saturated solution was extracted	(2) made from doubly distilled
with hexane and analyzed by gas chromatography.	water and salts 99+% pure.
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 1.8 (std. dev.)
	REFERENCES :
	<ol> <li>Lyman, J.; Fleming, R.H.;</li> <li><i>J. Mar. Res.</i> 1940. 3. 135.</li> </ol>
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